HNF-33512
Revision 0

Methodology for the Number of Filters Needed in a Waste Box

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Project Hanford Management Contractor for the
U.S. Department of Energy under Contract DE-AC06-96RL13200

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EDC #: HNF-EDC-07-33520

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Program/Project: SW

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Fluor Government Group

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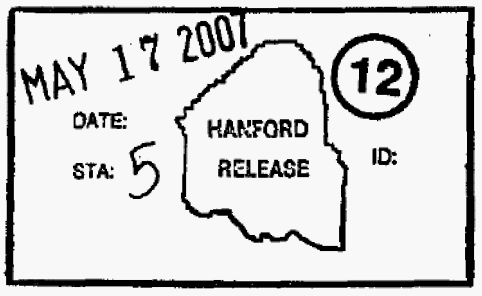

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Printed in the United States of America

Total Pages: 37

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Acronyms

FRP	Fiberglass Reinforced Plywood
LFL	lower flammability limit
MDSA	Master Documented Safety Analysis
PNNL	Pacific Northwest National Laboratory
QA	Quality Assurance
TRU	tranuranic
TSR	Technical Safety Requirements
VOC	volatile organic compounds

VOC Concentrations in Waste Box and the Number of Filters Necessary to Keep Concentration Low

1.0 INTRODUCTION

Waste in large waste boxes can generate volatile organic compounds (VOCs) and hydrogen. These waste boxes may or may not have flow paths out of them (although it is believed that most do). These boxes will be retrieved, sampled, and then coated with polyurea. After coating, filters will be installed in the box to keep the concentration of VOCs and hydrogen acceptably low. The MDSA requires that a vent path must be protected during application of the polyurea coating. If the box has been sampled then it is vented and the vent path must be protected.

This report provides a model in which the user inputs the free volume of the waste box, sample concentration (ppm of total VOC or volume fraction hydrogen) along with the number of filters to be placed into the waste box lid. Using this information, the model provides an estimate of concentration vs. time or the number of filters needed to reduce the concentration by a specified fraction. If the equations from this report are placed into spreadsheets which are then used to demonstrate TSR compliance, the spreadsheets must come under the Software QA Plan for such documents.

Chapters 2 and 3 present the theory. Chapter 4 presents the method with examples of its use found in Chapter 5. Chapter 6 provides the basis for the use of 1,000 ppm as the concentration below which the method is valid under any condition.

Conclusion

A model has been developed to equate the number of filters needed to be put into the waste box with the required decrease of concentration vs. time after the filters have been installed. The model requires the following knowledge:

- Use of the atmospheric breathing rate constant of 5.3×10^{-8}/s.
- Knowledge of the volume between the outer packaging and the inside walls of the box, is called the free volume. If unknown, a value of 0.5 times the interior volume of the empty container should be used.
- Resistance of the filters being used in the box after sealing and sampling. The resistances for the filters considered in this paper are:
    - 2,728 s/L for the NFT-015DS filter and 248 s/L for the NFT-016SSHP filter when passing hydrogen.
    - 27,280 s/L for the NFT-015DS filter and 2,480 s/L for the NFT-016SSHP filter when passing VOCs.
    - When more than one filter is used, the resistances above are divided by the number of filters.
- The resistance of the gaps present in the box during storage prior to retrieval. If unknown, a value of 7,800 s/L should be used, for calculations involving VOCs and 780 s/L for calculations involving hydrogen.

The first part of the method uses Equation 8 (See Section 3.2) and the sample results to obtain the generation rate. The second part of the method uses the generation rate obtained in Equation 8, the resistance of the filters being used, the initial sample concentration and Equation 4 (see Section 2.0 below) to obtain the time-varying moles (or concentration) in the box.

Alternatively, an estimate of the number of filters required to reduce the concentration to a desired fraction can be obtained. Equations 13a and 13b (Section 5.2) are used to estimate the number of filters needed to reduce the concentration to the desired value. The time necessary to reduce the concentration to the desired value is about 2 years after installation of the filters. If the time required to reach the desired ratio needs to be less than about 2 years, additional filters will be needed.

If the measured total VOC concentration is 1,000 ppm or below (the concentration below the saturation vapor pressure of all identified VOCs at 32 °F and above) or if the actual concentration of a known VOC is below its saturation vapor pressure, the method laid out in Section 5 can be used.

If the vapor pressure is above the saturation vapor pressure for the actual VOC in the waste box at the waste box temperature, the method outlined in Sections 4 and 5 cannot be used. Install a minimum of 4 filters in the waste box and monitor.

HNF-29785, *Action Concentration for Mixtures of VOCs, Methane and Hydrogen,* provides a requirement that if the VOC concentration exceeds 5,000 ppm, the sample should be further analyzed to determine the specific VOCs present. The reason for the difference between the 5,000 ppm criteria in HNF-29785 and the 1,000 ppm criteria here is that HNF-29785 was concerned with the lower flammability limit (LFL), whereas this report is concerned about determining a generation rate. To determine the generation rate it is important to know if the partial pressure of the VOC is at its saturation pressure. This is not important in determining the LFL because the LFL can be above or below the saturation pressure. As an example, the saturation vapor pressure for trimethyl benzene at 298 K is 0.0028 atm. This equates to a volume fraction of 0.0028. The LFL is 0.009 (data from Table 2). Trimethyl benzene vapors are not flammable below 298 K. On the other hand, the saturated vapor pressure of acetone is 0.3 atm (volume fraction of 0.3), where as the LFL is 0.026.

2.0 CONCENTRATION IN WASTE BOX AFTER RETRIEVAL AND PLACEMENT OF FILTERS

Once retrieved, assume the box needs to be coated with polyurea which would seal the box. Therefore, a filter will be installed and sampled. Using the results of the sample, use of this document will determine how many more filters will be needed to assure adequate venting or abatement of the flammable gas. After all filters have been installed, the box could then be polyurea coated. If the box were not sealed, the equation below would have to be modified to include the additional diffusion paths. For the purpose of this paper, the boxes are assumed to be coated so that the only diffusion, forced flow and breathing flow path is through the filters. The equation for the concentration in a sealed waste box with filters is as follows.

$$\frac{dM}{dt} = G - MQ - \frac{M}{VR_n} - \frac{GC_1}{V}M \qquad (1)$$

Where Q = atmospheric breathing rate constant, s^{-1} (see below)
= $(1.9 \times 10^{-4}/hr)/(3{,}600\ s/hr)$
= $5.3 \times 10^{-8}/s$
R_n = resistance of the filter(s), s/L (see below)
G = VOC or hydrogen generation rate, moles/s
M = mass of VOC or hydrogen present, moles
V = free volume of waste box outside the intact packaging, L
C_1 = Value of "L/mole" at the temperature of interest and 1 atm using the ideal gas law.

The equation and value of "Q" is taken from Appendix C of HNF-16166, *Required Staging Times for Hydrogen Diffusion in Vented Waste Containers.* This equation is used to determine the required number of filters, given an initial concentration.

The first term on the right hand side of the equation is the generation rate. The second term is removal of VOCs or hydrogen due to atmospheric breathing. Atmospheric breathing is forced flow into and out of the waste box via the filters due to changes in barometric pressure. Flow out due to diurnal temperature changes is not modeled thus conservatism to the calculation is introduced but not quantified. The third term is removal of VOCs or hydrogen due to diffusion through the filters. The last term is flow out due to the generation of gas.

Equation 1 is written for one component; either VOCs or hydrogen. If the waste box is generating/producing both VOC and hydrogen, the equation must be solved for each separately.

In the cases to be analyzed there are "n" filters used. The resistance of "n" filters, assuming the filters are all the same model, is given by

$$\frac{1}{R_n} = \frac{n}{R}$$

The only filters considered in this paper are either a Nucfil® model NFT-016SSHP or Nucfil® model NFT-015DS due to their lower resistances. (Nucfil® is a trademark of Nuclear Filter Technology). Other filters can be used, however. One just needs the diffusion parameter for these filters. The diffusion parameter from the manufacturer for diffusion of hydrogen through these filters is:

Model NFT-015DS: 1.5×10^{-5} moles/s-mole frac. (Appendix A of HNF-16166)
Model NFT-016 SSHP: 1.65×10^{-4} moles/s-mole frac.

The resistance for diffusion through a filter is derived in HNF-16166, Rev. 7, page B-3 (2006) and is given, in that reference, by:

$$\text{Resistance} = [(\text{moles/s-mole frac})(24.44)]^{-1}$$

or, using the terminology of this paper,

$$\text{Resistance} = [(DP)(C_1)]^{-1} \quad (2)$$

Using the above, the resistances of these filters for hydrogen diffusion are:

NFT-015DS:	2728 s/L for H_2
NFT-016SSHP:	248 s/L for H_2

When these filters pass VOCs, the resistance must be increased. This is because Appendix B of HNF-16166 shows that the diffusion parameter of the filter is inversely related to the diffusivity of the gas or vapor being passed. Section 2.1 of HNF-25634, *Potential For A Volatile Organic Compound (VOC) Deflagration In A TRU Drum*, shows that the diffusivity of hydrogen is 0.784 cm^2/s. The diffusivity of various VOCs range from 0.12 cm^2/s per acetone to 0.08 cm^2/s for trichloroethane. The "worst case" ratio of the diffusivities is a factor of 10. Therefore, in this analysis the diffusion parameter must be increased by a factor of 10 when VOCs are being passed. This results in a resistance that is a factor of 10 greater per Equation 2. Equation 2 can now be generalized to:

$$\text{Resistance} = \frac{VOCM}{DP * C_1}$$

The resistance of these filters when passing VOCs is then

NFT-015DS:	27,280 s/L for VOCs
NFT-016SSHP:	2,480 s/L for VOCs

Equation 1 will now be solved. Simplify Equation 1 to read:

$$\frac{dM}{dt} = G - \alpha M \quad (3)$$

Where $\alpha = \left(Q + \frac{1}{VR_n} + \frac{GC_1}{V} \right)$. The term "$\alpha$" is the overall removal rate constant and has units of sec^{-1}.

Assume at t = 0, M = M_o, where M_o is the quantity of VOC or hydrogen (in units of moles) present at the time the sample is taken. It is assumed that the filters are inserted within a few days or less after taking the sample.

The solution is

$$M = \frac{G}{\alpha}\left[1 - e^{-\alpha t}\right] + M_o e^{-\alpha t} \quad (4)$$

If the sample result provides the concentration in parts per million by volume (called C_{ppm}), which is typical for VOCs, then

$$M_o = \frac{(C_{ppm})\,V}{(10^6)(C_1)} \tag{5}$$

If the sample result provides the concentration in terms of a volume fraction (called C_{vf}), which is typical for hydrogen, then

$$M_o = \frac{(C_{vf})\,V}{C_1} \tag{6}$$

The free volume outside of the packaging for drums is 0.5 times the drum volume. (Section 3.1 of HNF-16166). That same free volume will be used in this analysis. If there is reason to believe the free volume is larger, a greater value should be used.

With the free volume and filter resistance now known, the overall removal rate constant, α, can be calculated. The only variable remaining is the generation rate, "G". Once "G" is obtained, Equation 4 can be solved to determine the number of filters required to bring the initial concentration down to a target concentration in a time period of interest.

3.0 GENERATION RATE

This section will provide a basis for a choice of a generation rate. What is desired is the greatest generation rate that produces a given sample result. This will result in the longest times to decrease to a certain concentration after the filters are added. The greatest generation rate that produces a given sample result is found when the box has leakage. Leakage allows diffusion to occur more readily, allows atmospheric breathing and allows forced flow.

3.1 HYDROGEN GENERATION

Section 3 of HNF-16166 shows that for the case where a waste drum contained 200 g of a 12% ^{240}Pu mixture with 1.7% ^{241}Am (radionuclide distribute taken from Table D-1 of HNF-16166), the generation rate has a maximum of 2.66×10^{-8} moles/s, assuming that 100% of the radionuclides are located on a reasonably bounding hydrogenous material (polyethylene). This generation rate is modified by a factor of "f", which is the fraction of radionuclides actually in intimate contact with this bounding hydrogenous material. Section 3 of HNF-16166 uses a value of 0.5 based on a Pacific Northwest National Laboratory (PNNL) report.

The hydrogen generation rate for 200 g TRU is 1.33×10^{-8} moles/s (obtained from multiplying 2.66×10^{-8} times 0.5, where 0.5 is the value for "f" discussed in the paragraph above). The hydrogen generation rate can be scaled using the number of grams of plutonium actually present in the waste box.

3.2 VOC GENERATION

Obtaining the generation rate for VOCs is more difficult as the generation rate depends on:

- VOC(s) present,
- thickness and type of packaging between VOC and free volume,
- temperature in waste box, and
- VOC concentration in the free space.

Little to none of the above information is known. Therefore, a different approach is needed. It should be noted that this method could also be used for hydrogen with the appropriate modifications. This would not typically be done as the hydrogen generation rate has been set by precedent at the value in Section 3.1.

The waste box may or may not have a gap or opening between the lid and the walls. If the gap exists, the worst case long term, volumetric flow rate due to pressure gradient would be equal to the volumetric generation rate of the VOC (and hydrogen if produced as well). A flow rate of this size would maintain the box at equilibrium.

The volumetric flow rate of the VOC is given by

$$V_G = (G)(C_I).$$

Large gaps also create large diffusion paths. Appendix C of HNF-16166 shows that

$$R = \frac{x}{AD}$$

Where x = length of the diffusion path, cm
A = cross-sectional area of diffusion path, cm^2
D = diffusivity, cm^2/s
= 0.08 cm^2/s for VOCs

The approach will be to assume there are gaps in the box through which flammable gases could escape while in storage (and before filter installation). Therefore, a worst case gas generation will be calculated.

A typical Hanford fiberglass reinforced plywood waste box is made of an exterior surface of ¾ inch plywood, 2 x 8 frame and interior ¾ inch plywood (from Section 2.2 of HNF-26310, *Fiberglass Reinforced Plywood (FRP) Container Storage*). Assuming a 2 x 8 is 7.5 inches long, the path length in this case, is 9 inches (from 7.5 inches for the "2 x 8" and 1.5 inches for the plywood covering). For other cases it is less.

The boxes have a gasket between the lid and the body. Assume there are openings in that gasket (gaskets are normally installed in pieces). Assume a gap height of ¼ inch (0.64 cm) (about the height of a gasket prior to being compressed). Assume a length in the direction of

flow of 4 inches (10.2 cm). Assume a width of 0.25 inches each for 4 gaps. This is a total gap width of 1 inch (2.54 cm). These values are on the conservative side of "typical" and are chosen to assess sensitivity. The resistance, assuming VOCs are diffusion, is

$$R = \frac{10.2\ cm}{(0.64\ cm)(2.54\ cm)(0.08\ cm^2/s)}$$
$$= 78\, s/cm^3$$
$$= 78{,}000\ s/L$$

The approach taken is to relate the generation rate to the concentration found in the sample of the waste box free space. The equation to be solved is similar to Equation 1 but the diffusion and atmospheric breathing path is through gaps in the waste box between the lid and the body not through the filters.

The equation that will be solved is the following:

$$\frac{dM}{dt} = G - MQ - \frac{GC_1}{V}M - \frac{M}{VR_g} \qquad (7)$$

Where C_1 = 24.44 L/mole at 1 atm and 298 K per the ideal gas law per HNF-16166
V = free volume in waste box, L
= (20 ft long)(10 ft wide)(8 ft tall)(0.5)(28.3 L/ft^3)
= 22,640 L
R_g = resistance to diffusion flow through the gaps, s/L
= 7,800 s/L for calculations involving VOCs (see below)
Q = 5.3 x 10^{-8} sec^{-1}

The first term to the right of the equals sign is the generation rate. The second term is removal due to atmospheric breathing. The third term is removal due to volumetric flow resulting from generation. The last term is diffusion out of the gaps.

The storage time is long, about 20 yrs. Equation 4 presents the solution for Equation 7, where, in this case,

$$\alpha = \left(Q + \frac{1}{VR_g} + \frac{GC_1}{V}\right)$$

In this case,

Q = 5.3 x 10^{-8} s^{-1}
V = 22,640 L
R_g = 7,800 s/L
C_1 = 24.44 L/mole
M_o = 0 moles

If, "G" is 10^{-10} moles/s, then α is 5.9 x 10^{-8} s^{-1}. There are 6.3E+8 s in 20 years. Using Equation 4 and substituting these values results in the following:

$$M = \frac{G}{\alpha}\left[1 - e^{-\alpha t}\right] = \frac{G}{\alpha}$$

This result means that steady state has been achieved as the value of M does not change with time. Steady state is achieved for larger values of "G" and for smaller values. Steady state is also achieved for smaller volumes. It should be noted that for a value of α of 5.9 x 10^{-8} s^{-1} and a duration of 2.5 years (7.9 x 10^{7} s), the result of the equation above is 0.99 (G/α). The result is that the concentration is essentially at steady state conditions at 2.5 years.

Since at 20 years, steady state has been achieved, Equation 7 can be simplified to:

$$0 = G - M_o Q - \frac{G C_1}{V} M_o - \frac{M_o}{V R_g}$$

Solving for "G" yields

$$G = \frac{M_o\left(Q + \frac{1}{V R_g}\right)}{\left(1 - \frac{C_1 M_o}{V}\right)} \qquad (8)$$

Where M_o = moles in waste box per the sample (see Equations 5 and 6)

What we are trying to find is the generation rate for a specific free volume concentration based on "M".

For the calculation to follow, "R_g" is conservatively chosen to be 7,800 s/L. That is, the combined width of the openings is 10 inches not 1 inch as assumed above. If this method is used to determine hydrogen generation rate, then R_g is set at 780 s/L.

A spreadsheet was developed to calculate values for "G" using Equation 8. Table 1a provides the results for a waste box free volume of 22,640 L. Table 1b provides the results for a 4 ft by 4 ft by 7 ft box.

Table 1a. Generation Rate As A Function Of Sample Concentration in a Large Waste Box (VOC Diffusion)[1]

C_{ppm}, parts per million	M_o, Moles	Generation Rate, G
1	9.26E-04	5.43E-11
5	4.63E-03	2.72E-10
10	9.26E-03	5.43E-10
30	2.78E-02	1.63E-09
60	5.56E-02	3.26E-09
100	9.26E-02	5.43E-09
300	2.78E-01	1.63E-08
600	5.56E-01	3.26E-08
1,000	9.26E-01	5.44E-08
3,000	2.78E+00	1.64E-07
6,000	5.56E+00	3.28E-07
10,000	9.26E+00	5.49E-07
30,000	2.78E+01	1.68E-06
60,000	5.56E+01	3.47E-06
100,000	9.26E+01	6.04E-06
Note 1: Waste box is 20 ft by 10 ft by 8 ft. Free Volume is assumed to be 22,640 L based on a free fraction of 0.5		

Table 1b. Generation Rate As A Function Of Sample Concentration in a Small Waste Box (VOC Diffusion)[1]

C_{ppm}, parts per million	M_o, Moles	Generation Rate, G
1	6.49E-05	8.68E-12
5	3.24E-04	4.34E-11
10	6.49E-04	8.68E-11
30	1.95E-03	2.60E-10
60	3.89E-03	5.21E-10
100	6.49E-03	8.68E-10
300	1.95E-02	2.61E-09
600	3.89E-02	5.21E-09
1,000	6.49E-02	8.69E-09
3,000	1.95E-01	2.61E-08
6,000	3.89E-01	5.24E-08
10,000	6.49E-01	8.77E-08
30,000	1.95E+00	2.69E-07
60,000	3.89E+00	5.54E-07
100,000	6.49E+00	9.65E-07
Note 1: Waste box is 4 ft by 4 ft by 7 ft. Free Volume is assumed to be 1585 L based on a free fraction of 0.5		

3.3 INCREASE IN NUMBER OF MOLES PRESENT

There may be a situation when the filters cannot be added to the waste box immediately after retrieval. A "worst-case" assumption would be that the waste box being retrieved is sealed (waste boxes are assumed to have gaps that allow for diffusion and forced flow of hydrogen and VOCs out) or that it is successfully argued that the waste box can be coated (i.e., sealed) and then placed in storage for a period of time before the filters are added. In addition, it is further assumed that no sample was taken during this time. Under these conditions the concentration will increase above that at retrieval. This section shows the ratio of the final concentration to that at the time the waste box is retrieved.

The concentration at the time when the waste box is retrieved is

$$C_o = \frac{M_o}{M_o + M_a} = \frac{M_o}{M_{t,o}}$$

Where M_o = moles of hydrogen or VOC in waste box
M_a = moles of air in the waste box
$M_{t,o}$ = total moles in waste box
$= V/C_1$.

At a later time after retrieval the waste box,

$$C = \frac{M_o + G\Delta t}{M_{t,o} + G\Delta t}$$

Where G = generation rate, moles/s
Δt = duration from time of retrieval, s

The ratio of the concentration at a later time over that at the time of retrieval is

$$\frac{C}{C_o} = \left(\frac{M_o + G\Delta t}{M_{t,o} + G\Delta t}\right)\left(\frac{M_{t,o}}{M_o}\right) = \frac{1 + \frac{G}{M_o}\Delta t}{1 + \frac{G}{M_{t,o}}\Delta t}$$

From Equation 8

$$\frac{G}{M_o} = Q + \frac{GC_1}{V} + \frac{1}{VR_g}$$

Substituting yields

$$\frac{C}{C_o} = \frac{1 + \left(Q + \frac{GC_1}{V} + \frac{1}{VR_g} \right) \Delta t}{1 + \frac{G}{M_{t,o}} \Delta t} \qquad (8a)$$

The results will be shown next.

Using the data and definitions in Section 3.2,

V = 22,640 L (the large waste box)
R_g = 7800 s/L
Q = 5.3 x 10^{-8} s^{-1}
C_1 = 24.44 L/mole
$M_{t,o}$ = V/C_1

Let Δt = 30 days or 2.59 x 10^6 s. Choosing values of G based on Tables 1a and 1b, the following is found:

V = 22,640 L		V = 1,585 L	
G, moles/s	**C/C_o**	**G, moles/s**	**C/C_o**
10^{-11}	1.15	10^{-11}	1.35
10^{-10}	1.15	10^{-10}	1.35
10^{-9}	1.15	10^{-9}	1.35
10^{-8}	1.15	10^{-8}	1.35
10^{-7}	1.15	10^{-7}	1.35
10^{-6}	1.15	10^{-6}	1.33

To use the methodology, assign a value of 10^{-6} moles/s to "G" and solve the equation 8a above.

4.0 METHODOLOGY FOR DETERMINING THE VOLUME FRACTION VS. TIME AFTER THE FILTERS HAVE BEEN INSTALLED

The following are the steps of the methodology:

1. Obtain concentration reading in parts per million (C_{ppm}) or volume fraction (C_{VF}) from the sample.
2. Determine free volume of box (V)
3. Obtain M_o from either
$$M_o = (C_{ppm})(10^{-6})(V)/(C_1)$$
$$M_o = (C_{VF})\ V/C_1$$
4. Set "R" = 7,800 s/L for VOC diffusion and 780 s/L for hydrogen diffusion.
5. Set "Q" = 5.3 x 10^{-8} sec^{-1}
6. Calculate the generation rate from the concentration using Equation 8 for VOCs or use the generation rate given in Section 3.1 for hydrogen.
7. With "G" from Step 6, solve Equation 4 with

$$\alpha = Q + \frac{1}{VR_n} + \frac{GC_1}{V}$$

Where $Q = 5.3 \times 10^{-8}$ sec^{-1}

R_n = based on number of filters, the filter type (see Section 2) and whether hydrogen or VOC is being removed.

Start by choosing a filter type and number of filters. Determine the concentration in the waste box as a function of time. If the concentration decreases too slowly, assume additional filters or choose a different filter.

5.0 EXAMPLES

5.1 EXAMPLE OF THE METHOD THAT PROVIDES THE CONCENTRATION OVER TIME AFTER FILTERS HAVE BEEN INSERTED (VOC DIFFUSION)

All of the examples are based on VOCs.

Step 1 – Assume sample result is 10,000 ppm.
Step 2 – Assume waste box is 20 ft by 10 ft by 8 ft with 0.5 of it void (volume fraction outside packaging). V = 22,640 L
Step 3 – Using the equation $M_o = (C_{ppm})(10^{-6})(V)/(C_1)$, M_o is found to be 9.26 moles when C_1 is 24.44 L/mole
Step 4 – Set R = 7,800 s/L
Step 5 – Set $Q = 5.3 \times 10^{-8}$ s^{-1}
Step 6 – Using Equation 8, G is found to be 5.5×10^{-7} moles/s
Step 7 – From above
$M_o = 9.26$ moles
$G = 5.5 \times 10^{-7}$ moles/s
Assume four NFT-015DS filters.
$R_{NFT\text{-}015DS} = 27{,}280$ s/L for each filter for VOCs
$R_n = 6{,}820$ s/L for four filters
V = 22,640 L for the large waste box
$\alpha = Q + (VR)^{-1} + (G\,C_1/V)$
$= 6.0 \times 10^{-8}$ s^{-1}

Solve Equation 4 to obtain a value for "M". Then determine the concentration (in ppm) from the following:

$$C_{ppm} = (10^6)*M*(C_1)/V$$

Table 2, Column 2 provides the results.

The volume fraction does not change, so a change in either the number of filters or type needs to be made if the required diffusion needs to be changed. First assume eight NFT-015DS filters. Now "R_n" is 3,410 s/L. Solve Equation 4. The results are in Column 3 of Table 2.

The volume fraction still does not change much so choose four NFT-016SSHP filters. Now $R_{NFT\text{-}016SSHP}$ = 2,480 s/L and R_n = 620 s/L. The results are shown in the last column of Table 2.

Results of the method for a waste box having a free volume of 22,640 L, M_o = 9.26 moles

Table 2. Concentration in Large Waste Box Over Time (10,000 ppm, initially)

Time, days	Concentration of VOC in box with 4 NFT-015DS filters, ppm	Concentration of VOC in box with 8 NFT-015DS filters, ppm	Concentration of VOC in box with 4 NFT-016SSHP filters, ppm
0	10,000	10,000	10,000
2	10,000	9990	9890
14	10,000	9920	9270
30	9990	9830	8550
60	9970	9690	7500
180	9930	9310	5510
365	9990	9060	4860
730	9890	8940	4760
1096	9890	8930	4760
2190	9890	8930	4760
Based on free volume "V", V=22,640 L, M_o = 9.26 moles (C_{ppm} = 10,000 ppm), C_1 = 24.44 L/mole and VOC diffusion			

Large Waste Box, 1,000 ppm Initial Concentration

For purposes of comparison, substitute 1,000 ppm for step 1 above. In this case

- Step 3 shows that M_o = 0.926 moles
- Step 6 shows that G = 5.4 x 10^{-8} moles/s

Table 3 provides the results from Step 7 assuming a large waste box and 1,000 ppm as the sample concentration.

Table 3. Concentration in Large Waste Box Over Time (1,000 ppm, initially)

Time, days	Concentration of VOC in box with 4 NFT-015DS filters, ppm	Concentration of VOC in box with 8 NFT-015DS filters, ppm	Concentration of VOC in box with 4 NFT-016SSHP filters, ppm
0	1000	1000	1000
2	1000	1000	990
14	1000	990	930
30	1000	980	850
60	990	970	750
180	990	930	550
365	980	900	480
730	980	885	470
1096	980	884	470
Based on free volume "V", V=22,640 L, M_o = 0.926 moles (1,000 ppm) C_1 = 24.44 L/mole and VOC diffusion			

Small Waste Box, 1,000 ppm Initial Concentration

To address the impact of a small waste box, use the 1,000 ppm case with a waste box volume of 1,585 L (4 ft by 4 ft by 7 ft waste box with 0.5 free fraction). In this case,

- Step 3 shows that M = 0.065 moles
- Step 6 shows that G = 8.7×10^{-9} moles/s

The results from step 8 are shown in Table 4

Table 4. Concentration in Small Waste Box Over Time (1,000 ppm initially)

Time, days	Concentration of VOC in box with 4 NFT-015DS filters, ppm	Concentration of VOC in box with 8 NFT-015DS filters, ppm	Concentration of VOC in box with 4 NFT-016SSHP filters, ppm
0	1000	1000	1000
2	1000	980	850
14	990	890	360
30	980	800	180
60	960	690	130
180	930	570	130
365	922	564	130
730	921	564	130
Based on free volume "V", V=1,585 L, M_o = 0.065 moles (1,000 ppm) C_1 = 24.44 L/mole and VOC diffusion			

5.2 METHOD THAT ARRIVES AT THE NUMBER OF FILTERS NEEDED TO REDUCE THE CONCENTRATION TO A SPECIFIED AMOUNT

In this section a method is developed to determine the number of filters necessary to reduce the concentration within the waste box such that $M/M_o = r$ in a waste box having a free volume outside the intact packaging of "V" liters and filters of a specific type.

Equation 4 is reproduced here:

$$M = \frac{G}{\alpha}(1 - e^{-\alpha t}) + M_o e^{-\alpha t}$$

At long times ($\alpha t > 5$, which occurs after about 2.5 years per Section 3.2) after the filters have been put in:

$$M = \frac{G}{\alpha} = \frac{G}{\left(Q + \frac{1}{R_n V} + \frac{GC_1}{V}\right)} \tag{9}$$

Note that "long times" means that essentially steady state conditions (the generation rate is essentially equal to the removal rate such that the concentration changes little with time) have been achieved.

At the time the filters are installed, $M = M_o$.

Since the filters are placed into the waste box after a long time of generation, dM/dt in Equation 7 can be set equal to zero. The modified Equation 7 can be rearranged to yield:

$$M_o = \frac{G}{\left(Q + \frac{GC_1}{V} + \frac{1}{VR_g}\right)}$$

The ratio of M/M_o is

$$\frac{M}{M_o} = \frac{\left(Q + \frac{GC_1}{V} + \frac{1}{VR_g}\right)}{\left(Q + \frac{1}{R_n V} + \frac{GC_1}{V}\right)} \tag{10}$$

Assume that a given ratio of M/M_o is required. Call this ratio "r". Then

$$r = \frac{\left(Q + \frac{GC_1}{V} + \frac{1}{VR_g}\right)}{\left(Q + \frac{1}{R_n V} + \frac{GC_1}{V}\right)}$$

After rearranging, the resistance of the set of filters needed to bring the ratio of M/M_o to "r" is:

$$\left(\frac{1}{R_n}\right) = \left(\frac{V}{r}\right)\left[Q(1-r) + \frac{GC_1}{V}(1-r) + \frac{1}{VR_g}\right] \tag{11}$$

Recall that,

$$\frac{1}{R_n} = \frac{n}{R}$$

Or

$$R_n = \frac{R}{n}$$

Also recall that

$$R = (VOCM) * [(DP)(C_1)]^{-1} \tag{12}$$

Where VOCM = 10 when the filters pass VOCs
= 1 when the filters pass hydrogen.
DP = diffusion parameter for the filter of interest, moles/s-mole frac.

Solving for "n", the number of filters needed yields

$$n = \frac{R}{R_n}$$

Substituting Equations 11 and 12 yields

$$n = \left(\frac{VOCM}{DP * 24.44}\right)\left(\frac{1}{R_n}\right) \tag{13a}$$

$$\left(\frac{1}{R_n}\right)=\left(\frac{V}{r}\right)\left[Q(1-r)+\frac{GC_1}{V}(1-r)+\frac{1}{VR_g}\right] \quad (13b)$$

Where n = number of filters needed to reduce the concentration by a ratio of "r" from the initial concentration
G = generation rate, moles/s
r = M/M_0 that is desired. That is the reduction of moles in the box from that initially
M_0 = moles of VOC or hydrogen in the waste box when the filters are put in.
M = moles of VOC or hydrogen at a later time.
Q = atmospheric breathing rate, 5.3×10^{-8} sec^{-1}
V = volume outside intact packaging, L
VOCM = 10 when the calculation is for VOCs
= 1 when the calculation is for hydrogen
R_g = resistance of gap in waste box between lid and body prior to coating, s/L
= 780 s/L for calculations involving hydrogen (see Section 3.2)
= 7,800 s/L for calculations involving VOCs (see Section 3.2)
DP = diffusion parameter for the filter of interest, moles/s- mole frac.
C_1 = value of L/mole at the temperature of interest and 1 atm
= 24.44 L/mole, if the temperature is 298 K.

In other words, based on Equations 13a and 13b above, "n" is the number of filters necessary to reduce the concentration within the waste box such that $M/M_o = r$ in a waste box having a free volume outside the intact packaging of "V" liters and filters of a specific type.

To determine the time necessary to reach the ratio "r", Equation 4 must be solved. The times are typically "many months" see Tables 2-4 for estimates.

Consider the case used to generate Table 2.

M_o = 9.26 moles (based on 10,000 ppm).
G = 5.5×10^{-7} moles/s.
Q = 5.3×10^{-8} moles/s.
V = 22,640 L
VOCM = 10
DP = 1.5×10^{-5} for the NFT-015DS filter.

Table 2 shows that 8 filters are necessary to reduce the volume fraction from 0.01 to 0.00893 in 1,096 days. The duration is chosen as the time at which steady state conditions are reached as this is the basis for Equations 13a and 13b. Therefore, to check the method, substitute 0.893 for "r" and solve for "n". Doing this, "n" is found to be 8.

Consider the conditions that result in the last column in Table 2. In this case,

M_o = 9.26 moles (based on 10,000 ppm)
G = 5.4×10^{-7} moles/s

$Q = 5.3 \times 10^{-8}$ moles/s
V = 22,640 L
VOCM = 10
$DP = 1.65 \times 10^{-4}$ for the NFT-016SSHP filter.

Table 2 shows that 4 filters are necessary to reduce the volume fraction from 0.01 (10,000 ppm) to 0.00476 (4,760 ppm) in 730 days. Therefore, to check the method, substitute 0.476 for "r" and solve for "n". Doing this, "n" is found to be 4.

If, NFT-015DS filters were to be used, it would take 44 filters to bring the volume fraction down to 0.00476.

One needs to be aware that when using this method of directly determining the number of filters, the time needed to reach the volume fraction of interest will likely be long (order of years). If this duration is too long, installation of additional filters may reduce the time needed. The effectiveness of additional filters can be determined using the method in Section 5.1.

6.0 DERIVATION OF 1,000 PPM AS THE CONCENTRATION BELOW WHICH THE MODEL CAN BE USED UNDER ANY CONDITIONS

This method only works if the concentration in the waste box when retrieved is below the saturation vapor pressure for the VOC of interest. This is because the generation rate is essentially zero when the concentration reaches the saturation vapor pressure.

Table 5 presents a list of the potential VOCs that could be found in waste containers. The first 29 entries come from HNF-25634. The last 11 entries came from recent sample data. Table 5 is located at the end of the report.

Using Table 5, at 298 K, the VOCs having the lowest vapor pressure are:

1,2,4 – trimethylbenzene	0.0031 atm
o-xylene	0.0087 atm
butanol	0.0087 atm

Since waste boxes experience a variety of temperatures, the saturated vapor pressure at other temperatures is required. The vapor pressure data comes from the DIPPR (2005), *Project 801-Evaluated Standard Thermophysical Property Values* (American Institute of Chemical Engineers).

The equation for vapor pressure is

$$Y = \exp\left[A + \frac{B}{T} + C(\ln t) + DT^{E}\right] \qquad (14)$$

Where T = temperature, K
Y = vapor pressure, Pa

The data to solve Equation 14 follows. The data for 2-methyl 2 butanol (t-amyl alcohol) is added, see below.

	A	B	C	D	E
1-butanol	107.09	-9914.7	-11.768	1.0925E-17	6
o-xylene	90.405	-7955.2	-10.086	5.9594E-6	2
1,2,4-trimethyl benzene	85.301	-8215.9	-9.2166	4.7979E-6	2
2-methyl 2 butanol	100.75	-9184.1	-10.924	2.8079E-17	6

The results are as follows:

	Vapor Pressure, atm (Note 1)		
VOC	273 K (32 °F)	319 K (115 °F)	298 K (77 °F)
1-butanol	0.0012	0.0351	0.0087
o-xylene	0.0017	0.0273	0.0087
1,2,4-trimethylbenzene	0.0005	0.0098	0.0028
2-methyl 2-butanol (t-amyl alcohol)	0.0034	0.0787	0.0217

Note 1: to obtain C_{ppm}, multiply the values by 10^6.

The data above is "actual" concentration. To get the measured concentration corresponding to this, the following must be solved.

Actual concentration = (measured concentration) * (correction factor)

The measured concentrations at 273 K (32 °F) are shown next. Since the correction factor for t-amyl alcohol is very large, it is added to the list as its measured concentration is the same order as the other three VOCs.

	Correction Factor	Measured Concentration, C_{ppm}
1-butanol	0.78	1,500
o-xylene	0.22	7,700
1,2,4-trimethylbenzene	0.17	2,900
2-methyl 2-butanol (t-amyl alcohol)	2.8	1,200

That is, if one measures a concentration, at 32 °F, of 2-methyl 2 butanol of 0.0012 atm or 1,200 ppm, (actual concentration is 0.0034 atm [3,400 ppm]), saturation conditions are reached.

What that means is that if the measured concentration in the waste box is 1,000 ppm or less, saturation conditions are never reached above 32 °F. At 77 °F (298 K), the saturation conditions are not reached as long as the concentration does not exceed 7,700 ppm. If temperatures never went below 77 °F, one could use 7,700 ppm instead of 1,000 ppm.

7.0 CONCLUSIONS

If the measured total VOC concentration is 1,000 ppm or below (the concentration below the saturation vapor pressure of all identified VOCs at 32 °F and above) or if the actual concentration of a known VOC is below its saturation vapor pressure, the method outlined in Section 5 **can** be used.

If the vapor pressure is above the saturation vapor pressure for the actual VOC in the waste box at the waste box temperature, the method outlined in Sections 4 and 5 **cannot** be used. Put 4 filters in the waste box and monitor.

8.0 STRATIFICATION

This calculation involves determining the VOC concentration as a function of location and time in a very large box to determine if VOC will be completely mixed within the free volume of that box. If the VOC mixes in the free volume of the waste box over a short period of time, the free volume can be modeled as well-mixed.

The interior of the large waste box is assumed to be 20 ft long, 10 ft wide and 8 ft tall. To be conservative, the VOC generator is assumed to be 6 ft beneath the top of the box and covering the entire base of the waste box.

The condition within the volume can be viewed as a rectangular free space with a planar VOC source generating VOC at the lower plane. This is a conservative condition in that typically the box contains a piece of equipment from which the VOC evaporates. The VOC source is then 3-dimensional rather than 2-dimensional as in the analysis. Also, there is typically not ¾ of the box height free as is assumed in this analysis.

The model allows for the fact that the VOC may (although not likely due to the small generation rate) initially stratify in the bottom of the waste box. Should this occur, the VOC concentration gradient will lessen as diffusion transports VOC from the stratified layer into the layer having a smaller VOC concentration.

The text, *The Mathematics of Diffusion*, Section 4.3.7 (1975) provides an equation to calculate the concentration within a volume defined by two parallel plates separated by a distance "2 l" and having a diffusing substance enter at a constant rate of "F_o" moles/s-cm^2 over the surface of each plate. The equation solved is

$$D \frac{\partial C}{\partial x} = F_o \quad \text{at } x = l$$

This is the condition posed by the VOCs in the waste box. The location "x = l" is the surface of the generator where "l" is the distance from the surface of the generator to the roof of the box. In this case "l" is 6 ft or 183 cm.

VOC is assumed to be generated at a rate of 10^{-7} moles/s.

The area for VOC generation is assumed to be the entire area of the waste box or

$$A = (10\ ft)(20\ ft\ long)(30.5\ cm/ft)^2$$
$$= 1.86 \times 10^5\ cm^2$$

The equation for hydrogen concentration in the IP-2 container as a function of location and time (from Section 4.3.7 of *The Mathematics of Diffusion)* is as follows:

$$C\text{-}C_o = \frac{F_o l}{D}\left[\frac{Dt}{l^2} + \frac{\left(3x^2 - l^2\right)}{6\,l^2} - \left(summation\ term\right)\right] \qquad (10)$$

Where C = concentration of VOC at time "t" and location "x," moles/cm^3

C_o = concentration of VOC at time equals zero and at all locations, moles/cm^3
= 0.0

F_o = VOC generation rate per unit area, moles/s-cm^2
= (10^{-7} moles/s)/1.86 x 10^5 cm^2
= 5.4 x 10^{-13} moles/cm^2-s

l = distance from surface of generator to top of the waste box, cm
= 183 cm

D = diffusivity of VOC in air, cm^2/s
= 0.078 cm^2/s

t = time, s

x = distance from a location midway between the plates to the point of interest, cm
= 0.0 in this case if the location is the roof of the IP-2 container
= "l" in this case if the point of interest is the top of the drums.

The summation term is

$$\frac{2}{\pi^2}\frac{(-1)^n}{n^2}\left[\exp\left(-D n^2 \pi^2 t / l^2\right)\right]\cos\frac{n\pi x}{l}$$

At large times (greater than about 5 hrs), this term is insignificant.

At time equals zero, C_o, the initial concentration in the free volume of the waste box is zero.

The equation for concentration is solved for points in time. For each of these cases, the first term of the equation is found from:

$$\frac{F_o l}{D} = \frac{\left(5.4 x 10^{-13}\ moles/cm^2 - s\right)(183\ cm)}{0.078\ cm^2/s} = 1.26 x 10^{-9}\ \frac{moles}{cm^3}$$

The concentration 20 hours after loading is now found.

At 20 hours after generation begins and for "x" equal to "l"

$$\frac{Dt}{l^2}+\frac{\left(3x^2-l^2\right)}{6\,l^2}=0.168+0.333=0.501$$

At 20 hours after generation begins and for "x" equal to 0

$$\frac{Dt}{l^2}+\frac{\left(3x^2-l^2\right)}{6\,l^2}=0.168-0.167=0.001$$

The concentration at 20 hours after generation begins (ignoring the summation term) is:

$C_{x=l} = 1.3 \times 10^{-12}$ moles/cm^3 (at roof)

$C_{x=o} = 6.3 \times 10^{-10}$ moles/cm^3 (at surface)

The VOC concentration at the roof (where "x" equals zero) is much smaller than it is near the surface of the generation ("x" equal to "l").

The concentration 100 hours after loading is now found.

At 100 hrs after generation begins, and for "x" equal to "l"

$$\frac{Dt}{l^2}+\frac{\left(3x^2-l^2\right)}{6\,l^2}=0.838+0.033=1.171$$

At 100 hrs after generation begins and for "x" equal to zero

$$\frac{Dt}{l^2}+\frac{\left(3x^2-l^2\right)}{6\,l^2}=0.838-0.167=0.671$$

At 100 hours after generation begins, the concentrations are:

$C_{x=l} = 8.5 \times 10^{-10}$ moles/cm^3 (at roof)

$C_{x=o} = 1.5 \times 10^{-9}$ moles/cm^3 (at surface)

The concentrations are about half.

Performing the same calculation at 600 hrs, the

Concentration at the roof 6.13×10^{-9} moles/cm^3
Concentration at the surface 6.8×10^{-9} moles/cm^3

At 600 hrs, the "well mixed" volume fraction is given by

$$Well\ Mixed\ Vol.\ frac. = \frac{(Gen.\ Rate)(3600\ s/hr)(Time, hr)(24.45\ L/mole)}{(Volume\ of\ waste\ box)} \quad (11)$$

The well-mixed volume fraction is 1.56×10^{-4}.

The result is now checked. The concentration calculated above should be the same as that found by multiplying the VOC generation rate by the total time elapsed and dividing by the volume of the waste open space. The amount of VOC generated in 600 hrs is

$$VOC = (10^{-7}\ moles/s)(600\ hr)(3600\ s/hr) = 0.216\ moles$$
$$V = (183\ cm\ tall)(1.86 \times 10^{5}\ cm^2) = 3.4 \times 10^{7}\ cm^3$$
$$C = VOC/V = 6.35 \times 10^{-9}\ moles/cm^3$$

The concentration gradient (found using the diffusion equation) yields the same concentration as using just a simple 1-volume model.

The concentration at 600 hours (25 days) is essentially uniform through the waste box assuming no transport out of the box. As a result, the volume of the waste container can be considered to be well mixed after about 600 hours.

9.0 REFERENCES

DIPPR, 2005, *Project 801-Evaluated Standard Thermophysical Property Values*, Design Institute for Physical Property Data/American Institute of Chemical Engineers, New York, New York.

HNF-16166, 2006, *Required Staging Times for Hydrogen Diffusion in Vented Waste Containers,* Rev. 7, Fluor Hanford, Inc., Richland, Washington.

HNF-25634, 2006.*Potential For A Volatile Organic Compound (VOC) Deflagration In A TRU Drum,* Rev. 0, Fluor Hanford, Inc., Richland, Washington.

HNF-26310, 2005, *Fiberglass Reinforced Plywood (FRP) Container Storage,* Rev. 0, Fluor Hanford, Inc., Richland, Washington.

HNF-29785, 2006, *Action Concentration for Mixtures of VOCs, Methane and Hydrogen,* Rev. 0, Fluor Hanford, Inc., Richland, Washington.

The Mathematics of Diffusion, 1975, Oxford Science Publications, New York, New York.

Table 5. Flammable VOCs and Gases found in TRU Waste Containers

Name	Mol. Formula	Mol. Wt. (g)	Lower Flammability Limits (mole %)	Correction Factor, Normalized to Propane	Vapor Pressure, at 298 K atm	Vapor Pressure divided by Correction Factor
acetone	C_3H_6O	58.1	2.6	0.78	0.30	0.385
hydrogen	H_2	2	4			
benzene	C_6H_6	78.1	1.4	0.33	0.124	0.376
butanol	$C_4H_{10}O$	74	1.4	0.78	0.00871	0.011
carbon disulfide	CS_2	76.13	1	0.24	0.473	1.971
chlorobenzene	C_6H_5Cl	112.6	1.3	0.22	0.0165	0.075
chloroethane (gas above 12°C)	C_2H_5Cl	64.5	3.6	0.61	--	
cyclohexane	C_6H_{12}	84.2	1.3	0.36	0.128	0.356
1,1-dichloroethane	$C_2H_4Cl_2$	99	5.4	<0.49	0.294	0.600
1,2-dichloroethane	$C_2H_4Cl_2$	99	6.2	0.33	0.10	0.303
1,2-dichloroethylene	$C_2H_2Cl_2$	97	9.7	0.19	0.44	2.316
1,1-dichloroethylene	$C_2H_2Cl_2$	96.9	7.3	0.44	0.79	1.795
Dichloromethane (methylene chloride)	CH_2Cl_2	85	15.5	0.49	0.57	1.163
dichloropropane	$C_3H_6Cl_2$	113	3.4	0.39	0.066	0.169
dioxane	C_4H_8O	88.1	2	0.6	0.049	0.082
ethyl benzene	C_8H_{10}	106.2	1.6	0.28	0.013	0.046
ethyl ether (diethyl ether)	$C_4H_{10}O$	74.0	1.9	0.5	0.66	1.320
isopropyl alcohol	C_3H_8O	60	2	1.5	0.066	0.044
methanol	CH_4O	32.05	7.3	1.4	0.164	0.117
methyl chloride (chloromethane) (gas above -24°C)	CH_3Cl	50.5	8.1	0.41	--	
methyl ethyl ketone	C_4H_8O	72	1.8	0.61	0.118	0.193
methyl isobutyl	$C_6H_{12}O$	100	1.3	0.33	0.026	0.079

Name	Mol. Formula	Mol. Wt. (g)	Lower Flammability Limits (mole %)	Correction Factor, Normalized to Propane	Vapor Pressure, at 298 K atm	Vapor Pressure divided by Correction Factor
ketone						
1,1,1-Trichloroethane	$C_2H_3Cl_3$	133.4	6.0	0.56	0.120	0.214
trichloroethylene	C_2HCl_3	131.4	8	0.24	0.090	0.375
1,2,4-trimethylbenzene	C_9H_{12}	120.2	0.9	0.17	0.0031	0.018
toluene	C_7H_8	92.2	1.2	0.28	0.038	0.136
o-xylene	C_8H_{10}	106.2	1	0.22	0.0087	0.040
m-xylene	C_8H_{10}	106.2	1	0.22	0.0109	0.050
p-xylene	C_8H_{10}	106.2	1	0.22	0.0117	0.053
Methylpentane (isohexane)	C_6H_{14}	86.2	1.0	Not found (assume 1.0)	0.28	0.280
Methylcyclopentane	C_6H_{12}	84.0	1	Not found (assume 1.0)	0.18	0.180
Hexane	C_6H_{14}	86.0	1.2	0.3	0.20	0.667
3-hexene	C_6H_{12}	84.0	1.2	0.44	0.20	0.455
Chlorobutane	C_4H_9Cl	92.0	1.8	Not found (assume 1.0)	0.11	0.110
t-amyl alcohol (2-methyl-2-butanol)	$C_5H_{12}O$	88	1.1	2.8	0.022	0.008
Propane	C_3H_8	44	2.1	1.0	1.0	1.000
Butane	C_4H_{10}	58	1.6	0.67	1.0	1.493
Dimethyl ether	C_2H_6O	46	3.4	1.4	1.0	0.714
Ethanol (ethyl alcohol)	C_2H_6O	46	3.3	1.7	0.053	0.031
Isobutane	C_4H_{10}	58	1.4	0.67	1.0	1.493

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APPENDIX A – TECHNICAL PEER REVIEW SHEET

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Desk Instruction 2.0, Rev. 1

CHECKLIST FOR TECHNICAL PEER REVIEW

Document Reviewed - **HNF-33512, Rev. 0**

Title: *VOC Concentration in Waste Box and the Number of Filters Necessary to Keep Concentration Low,* April, 2007, by Robert Marusich
Scope: whole document

Yes	No*	NA		
[✓]	[ ]	[ ]		Referenced analyses appropriate.
[✓]	[ ]	[ ]		Problem completely defined and all potential configurations considered.
[ ]	[ ]	[✓]		Accident scenarios developed in a clear and logical manner.
[✓]	[ ]	[ ]		Necessary assumptions explicitly stated and supported.
[ ]	[ ]	[✓]		Computer codes and data files documented.
[✓]	[ ]	[ ]		Data used in calculations explicitly stated in document.
[✓]	[ ]	[ ]		Data checked for consistency with original source information as applicable.
[✓]	[ ]	[ ]		Mathematical derivations checked including dimensional consistency of results.
[✓]	[ ]	[ ]		Models appropriate and used within range of validity, or use outside range of established validity justified.
[✓]	[ ]	[ ]		Hand calculations checked for errors. Spreadsheet results should be treated exactly the same as hand calculations.
[ ]	[ ]	[✓]		Software input correct and consistent with document reviewed.
[ ]	[ ]	[✓]		Software output consistent with input and with results reported in document reviewed.
[✓]	[ ]	[ ]		Limits/criteria/guidelines applied to analysis results are appropriate and referenced. Limits/criteria/guidelines checked against references.
[✓]	[ ]	[ ]		Safety margins consistent with good engineering practices.
[✓]	[ ]	[ ]		Conclusions consistent with analytical results and applicable limits.
[✓]	[ ]	[ ]		Results and conclusions address all points required in the problem statement.
[✓]	[ ]	[ ]		Format consistent with applicable guides or other standards.
[✓]	[ ]	[ ]	**	Review calculations, comments, and/or notes are attached.
[✓]	[ ]	[ ]		Document approved (for example, the reviewer affirms the technical accuracy of the document).

Paul D. Rittmann Paul Rittmann 4-16-07
Technical Peer Reviewer (printed name and signature) Date

* All "no" responses must be explained below or on an additional sheet.

** Any calculations, comments, or notes generated as part of this review should be signed, dated and attached to this checklist. The material should be labeled and recorded in such a manner as to be understandable to a technically qualified third party.

Reviewer notes for *VOC Concentration in Waste Box and the Number of Filters Necessary to Keep Concentration Low,* April, 2007, by Robert Marusich

(1) The concept of the approach to equilibrium is used in this report, but never quantified. Nearness to equilibrium should be an input parameter.

(2) The equation for number of filters uses intermediate results (i.e. G or number of moles) calculated from input quantities. The equations would be more useful if they included input parameters, such as the initial VOC concentration, or the desired steady state concentration.

Paul Rittmann Paul Rittmann 4-16-07

Reply to the Peer Review Comments:

(1) Changes were made on page 8 to better explain the concept of steady state. The discussion of steady state vs. non-steady state that was included at the end of Section 5 was removed. Instead, times were chosen (e.g., 1096 days, 730 days, etc) such that steady state conditions existed.
(2) A spreadsheet was developed to solve the equations developed in this paper. The spreadsheet uses input parameters, not intermediate results (like "G") to determine the number of filters required. In addition, the examples in Section 5.1 and 5.2 show how the input parameters are used to determine the intermediate results and the final result.

Robert Marusich 4/17/07